



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:36 AM UTC

PDB ID : 1R6U / pdb_00001r6u
Title : Crystal structure of an active fragment of human tryptophanyl-tRNA synthetase with cytokine activity
Authors : Yang, X.-L.; Otero, F.J.; Skene, R.J.; McRee, D.E.; Ribas de Pouplana, L.; Schimmel, P.
Deposited on : 2003-10-16
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

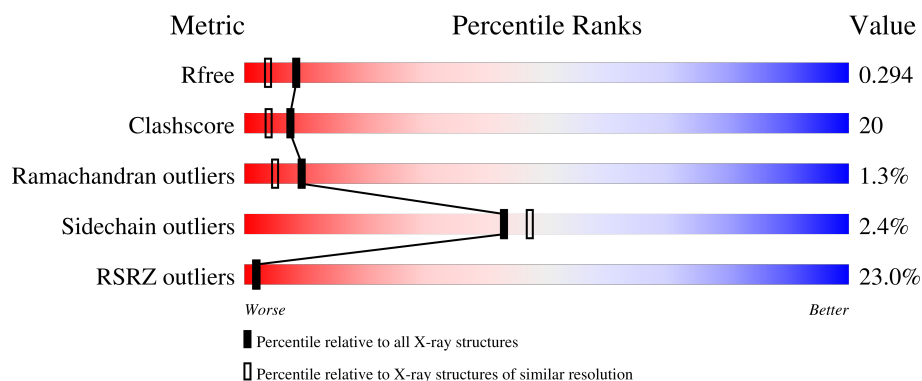
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	437	
1	B	437	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	601	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6205 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	Se	0	0	0
			3129	2004	528	582	5	10			
1	B	362	Total	C	N	O	S	Se	0	0	0
			2927	1879	497	537	5	9			

There are 50 discrepancies between the modelled and reference sequences:

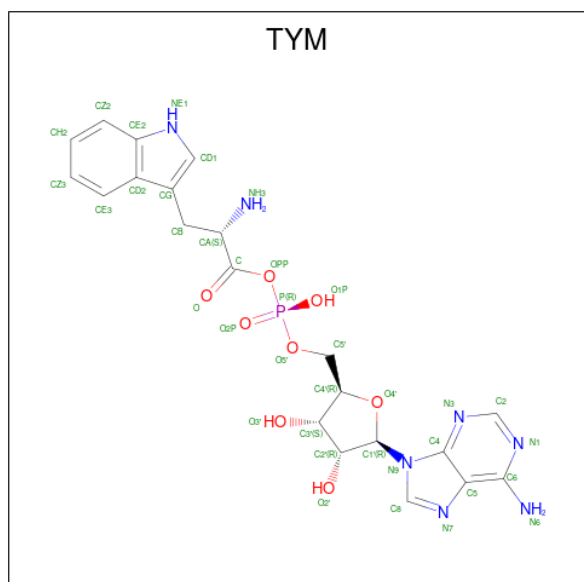
Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MSE	MET	modified residue	UNP P23381
A	169	MSE	MET	modified residue	UNP P23381
A	195	MSE	MET	modified residue	UNP P23381
A	213	GLY	SER	engineered mutation	UNP P23381
A	214	ASP	TYR	engineered mutation	UNP P23381
A	241	MSE	MET	modified residue	UNP P23381
A	243	MSE	MET	modified residue	UNP P23381
A	319	MSE	MET	modified residue	UNP P23381
A	350	MSE	MET	modified residue	UNP P23381
A	401	MSE	MET	modified residue	UNP P23381
A	425	MSE	MET	modified residue	UNP P23381
A	461	MSE	MET	modified residue	UNP P23381
A	472	LYS	-	cloning artifact	UNP P23381
A	473	LEU	-	cloning artifact	UNP P23381
A	474	ALA	-	cloning artifact	UNP P23381
A	475	ALA	-	cloning artifact	UNP P23381
A	476	ALA	-	cloning artifact	UNP P23381
A	477	LEU	-	cloning artifact	UNP P23381
A	478	GLU	-	cloning artifact	UNP P23381
A	479	HIS	-	expression tag	UNP P23381
A	480	HIS	-	expression tag	UNP P23381
A	481	HIS	-	expression tag	UNP P23381
A	482	HIS	-	expression tag	UNP P23381
A	483	HIS	-	expression tag	UNP P23381
A	484	HIS	-	expression tag	UNP P23381

Continued on next page...

Continued from previous page...

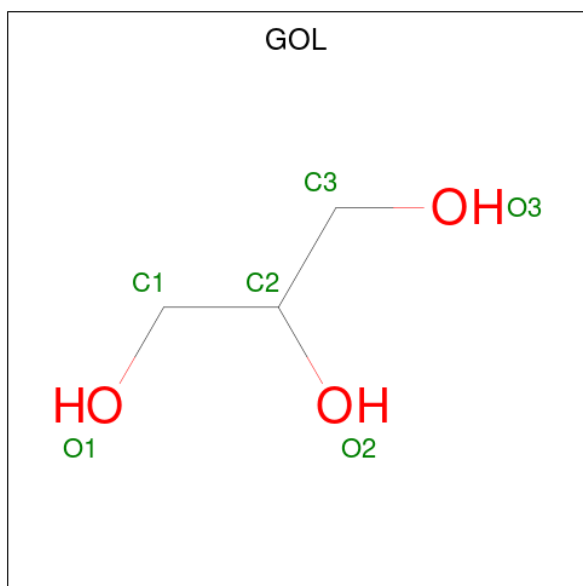
Chain	Residue	Modelled	Actual	Comment	Reference
B	143	MSE	MET	modified residue	UNP P23381
B	169	MSE	MET	modified residue	UNP P23381
B	195	MSE	MET	modified residue	UNP P23381
B	213	GLY	SER	engineered mutation	UNP P23381
B	214	ASP	TYR	engineered mutation	UNP P23381
B	241	MSE	MET	modified residue	UNP P23381
B	243	MSE	MET	modified residue	UNP P23381
B	319	MSE	MET	modified residue	UNP P23381
B	350	MSE	MET	modified residue	UNP P23381
B	401	MSE	MET	modified residue	UNP P23381
B	425	MSE	MET	modified residue	UNP P23381
B	461	MSE	MET	modified residue	UNP P23381
B	472	LYS	-	cloning artifact	UNP P23381
B	473	LEU	-	cloning artifact	UNP P23381
B	474	ALA	-	cloning artifact	UNP P23381
B	475	ALA	-	cloning artifact	UNP P23381
B	476	ALA	-	cloning artifact	UNP P23381
B	477	LEU	-	cloning artifact	UNP P23381
B	478	GLU	-	cloning artifact	UNP P23381
B	479	HIS	-	expression tag	UNP P23381
B	480	HIS	-	expression tag	UNP P23381
B	481	HIS	-	expression tag	UNP P23381
B	482	HIS	-	expression tag	UNP P23381
B	483	HIS	-	expression tag	UNP P23381
B	484	HIS	-	expression tag	UNP P23381

- Molecule 2 is TRYPTOPHANYL-5'AMP (CCD ID: TYM) (formula: $C_{21}H_{24}N_7O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			37	21	7	8	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

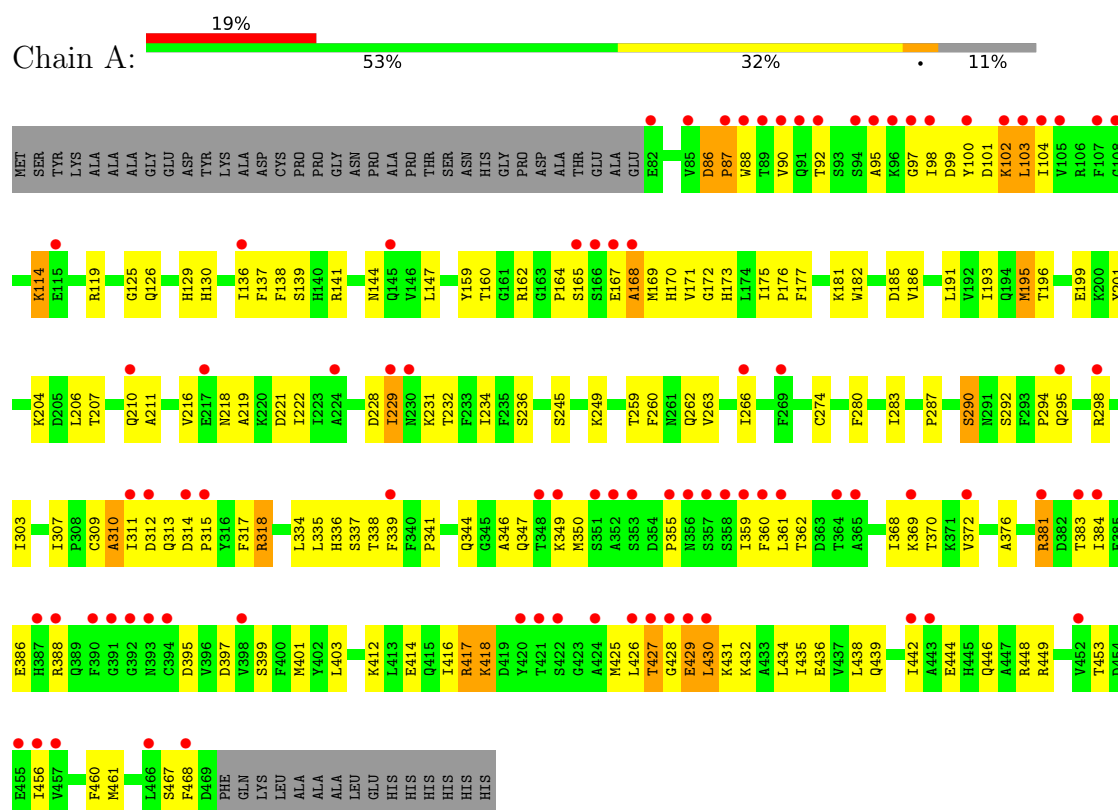
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	50	Total	O	0	0
			50	50		

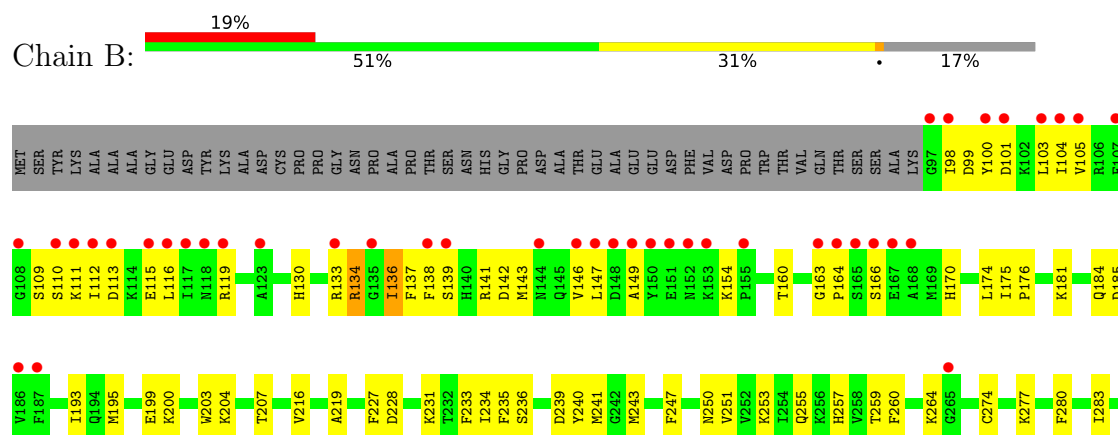
3 Residue-property plots

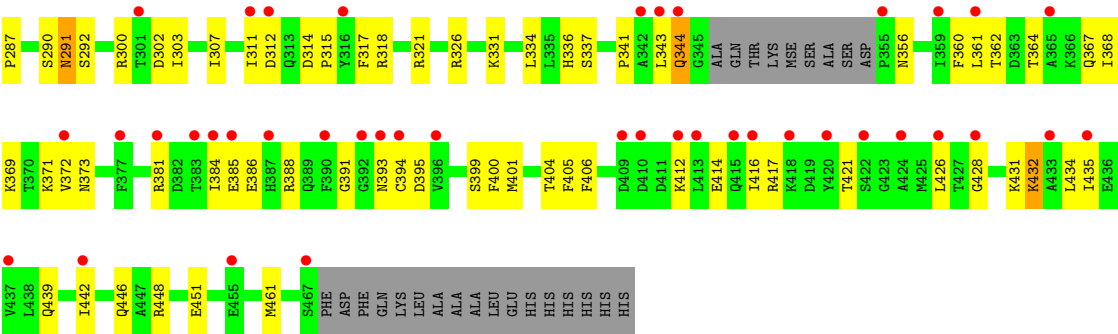
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tryptophanyl-tRNA synthetase



• Molecule 1: Tryptophanyl-tRNA synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.66Å 96.46Å 97.13Å 90.00° 129.90° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 93.6 (30.00-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.297 0.252 , 0.294	Depositor DCC
R_{free} test set	6233 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6205	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TYM, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/3195	1.01	9/4297 (0.2%)
1	B	0.42	0/2988	0.89	8/4014 (0.2%)
All	All	0.43	0/6183	0.95	17/8311 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	LEU	N-CA-C	-19.68	88.49	112.89
1	B	307	ILE	N-CA-C	9.35	117.41	108.15
1	A	427	THR	N-CA-C	-8.69	100.62	111.75
1	A	310	ALA	N-CA-C	-7.89	99.61	110.35
1	A	318	ARG	N-CA-C	-7.62	102.62	112.23
1	B	136	ILE	N-CA-C	-6.90	104.04	110.53
1	B	207	THR	N-CA-C	-6.49	101.79	110.55
1	A	136	ILE	N-CA-C	-6.38	104.27	110.72
1	A	102	LYS	N-CA-C	-6.28	106.16	113.88
1	B	290	SER	N-CA-C	6.10	118.72	111.33
1	B	292	SER	N-CA-C	-5.90	106.04	113.18
1	A	292	SER	N-CA-C	-5.87	105.96	113.01
1	A	103	LEU	N-CA-C	-5.62	105.92	112.89
1	B	406	PHE	N-CA-C	5.55	120.06	113.12
1	A	290	SER	N-CA-C	5.50	117.99	111.33
1	B	247	PHE	N-CA-C	5.43	116.89	110.97
1	B	166	SER	N-CA-C	-5.31	106.30	112.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3129	0	3075	134	0
1	B	2927	0	2893	113	0
2	A	37	0	23	3	0
3	A	12	0	14	2	0
4	A	50	0	0	4	0
4	B	50	0	0	3	0
All	All	6205	0	6005	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:GLU:HB3	1:A:432:LYS:HB2	1.18	1.12
1:A:95:ALA:HA	1:A:347:GLN:NE2	1.88	0.89
1:A:416:ILE:HA	1:A:425:MSE:HE1	1.56	0.86
1:B:250:ASN:HD21	1:B:291:ASN:ND2	1.74	0.86
1:B:143:MSE:HE3	1:B:146:VAL:HB	1.57	0.84
1:A:245:SER:O	1:A:249:LYS:HE2	1.81	0.80
1:B:250:ASN:HD21	1:B:291:ASN:HD21	1.32	0.77
1:B:241:MSE:HE1	1:B:283:ILE:HD12	1.68	0.75
1:A:206:LEU:HB2	1:A:210:GLN:HE21	1.52	0.75
1:A:432:LYS:O	1:A:436:GLU:HG3	1.86	0.75
1:A:312:ASP:HB3	1:A:339:PHE:CZ	2.23	0.74
1:B:174:LEU:HD21	1:B:361:LEU:HD21	1.69	0.73
1:B:253:LYS:O	1:B:257:HIS:HD2	1.71	0.73
1:B:141:ARG:HD3	1:B:321:ARG:NH1	2.03	0.72
1:A:95:ALA:HA	1:A:347:GLN:HE22	1.54	0.71
1:A:312:ASP:HB3	1:A:339:PHE:HZ	1.54	0.71
1:B:428:GLY:O	1:B:432:LYS:HG2	1.91	0.71
1:B:141:ARG:HD2	1:B:334:LEU:HD12	1.73	0.70
1:B:373:ASN:HA	1:B:431:LYS:HD3	1.71	0.70
1:A:137:PHE:CZ	1:A:337:SER:HB3	2.27	0.69
1:B:104:ILE:HG21	4:B:1080:HOH:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ILE:HB	1:B:176:PRO:HD3	1.74	0.69
1:B:448:ARG:O	1:B:451:GLU:HG2	1.93	0.69
1:A:169:MSE:HE3	1:A:221:ASP:HB2	1.74	0.68
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.59	0.67
1:A:309:CYS:SG	4:A:1087:HOH:O	2.52	0.67
1:B:251:VAL:O	1:B:255:GLN:HG3	1.95	0.66
1:A:429:GLU:C	1:A:432:LYS:H	2.04	0.66
1:A:90:VAL:HG23	1:A:349:LYS:HE3	1.78	0.65
1:A:181:LYS:HE2	1:A:185:ASP:OD2	1.96	0.64
1:A:229:ILE:HG12	1:A:460:PHE:CE1	2.32	0.64
1:B:112:ILE:HG23	1:B:116:LEU:HD23	1.80	0.64
1:A:310:ALA:HB3	1:A:312:ASP:OD1	1.99	0.63
1:B:300:ARG:HG2	1:B:300:ARG:HH11	1.62	0.63
1:B:104:ILE:HD11	1:B:111:LYS:N	2.14	0.62
1:A:429:GLU:HB3	1:A:432:LYS:CB	2.11	0.62
1:B:104:ILE:HD13	1:B:139:SER:HB3	1.82	0.62
1:B:321:ARG:O	1:B:331:LYS:HE3	2.00	0.61
1:A:336:HIS:CD2	4:A:1087:HOH:O	2.53	0.61
1:B:104:ILE:HD12	1:B:109:SER:OG	2.00	0.61
1:B:356:ASN:HA	1:B:371:LYS:HE2	1.82	0.61
1:B:369:LYS:HA	1:B:435:ILE:HD13	1.83	0.61
1:A:144:ASN:HB2	4:A:1034:HOH:O	2.01	0.61
1:A:418:LYS:HB2	1:A:418:LYS:NZ	2.15	0.61
1:B:112:ILE:HB	1:B:138:PHE:O	2.02	0.60
1:A:438:LEU:O	1:A:442:ILE:HG12	2.01	0.60
1:A:444:GLU:HB3	1:A:448:ARG:HH12	1.65	0.60
1:A:427:THR:O	1:A:428:GLY:C	2.44	0.60
1:A:442:ILE:O	1:A:446:GLN:HG3	2.01	0.60
1:B:384:ILE:HG23	1:B:385:GLU:OE2	2.02	0.60
1:B:113:ASP:OD1	1:B:115:GLU:HB3	2.02	0.59
1:B:234:ILE:O	1:B:461:MSE:HA	2.02	0.59
1:A:201:TYR:HA	1:A:206:LEU:HD11	1.84	0.59
1:B:181:LYS:HD3	1:B:185:ASP:OD2	2.02	0.59
1:A:171:VAL:HG23	1:A:359:ILE:O	2.02	0.59
1:B:119:ARG:HD3	1:B:147:LEU:HD13	1.86	0.58
1:B:101:ASP:O	1:B:104:ILE:HG22	2.03	0.58
1:A:100:TYR:C	1:A:102:LYS:H	2.11	0.58
1:A:137:PHE:CE1	1:A:337:SER:HB3	2.38	0.58
1:A:431:LYS:O	1:A:435:ILE:HG13	2.04	0.57
1:A:206:LEU:CB	1:A:210:GLN:HE21	2.18	0.56
1:A:100:TYR:O	1:A:101:ASP:HB3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:O	1:A:372:VAL:HG23	2.05	0.56
1:A:199:GLU:HB2	1:A:280:PHE:CZ	2.40	0.56
1:A:229:ILE:HD13	1:A:229:ILE:O	2.05	0.56
1:A:429:GLU:C	1:A:431:LYS:N	2.53	0.56
1:A:416:ILE:HG23	1:A:425:MSE:SE	2.55	0.55
1:A:274:CYS:HA	1:B:259:THR:HA	1.87	0.55
1:A:141:ARG:HG3	1:A:141:ARG:NH1	2.22	0.55
1:A:169:MSE:HA	1:A:173:HIS:ND1	2.21	0.55
1:B:137:PHE:CE1	1:B:337:SER:HB3	2.42	0.55
1:A:234:ILE:O	1:A:461:MSE:HA	2.06	0.55
1:B:442:ILE:O	1:B:446:GLN:HG3	2.07	0.55
1:B:139:SER:OG	1:B:311:ILE:HD13	2.07	0.54
1:B:104:ILE:HG12	1:B:111:LYS:HB2	1.89	0.54
1:B:203:TRP:CD1	1:B:277:LYS:HE2	2.43	0.54
1:A:453:THR:O	1:A:456:ILE:HB	2.09	0.53
1:A:164:PRO:HG3	1:A:195:MSE:HG3	1.89	0.53
1:B:98:ILE:HG21	1:B:100:TYR:HE2	1.73	0.53
1:B:136:ILE:HD12	1:B:405:PHE:CE1	2.44	0.53
1:A:307:ILE:HB	1:A:334:LEU:HD23	1.90	0.53
1:B:318:ARG:HG2	1:B:318:ARG:HH11	1.73	0.53
1:B:199:GLU:HB2	1:B:280:PHE:CZ	2.44	0.53
1:B:98:ILE:HG21	1:B:100:TYR:CE2	2.43	0.53
1:B:130:HIS:O	1:B:134:ARG:HB2	2.08	0.53
1:A:260:PHE:O	1:A:263:VAL:HG12	2.09	0.52
1:A:294:PRO:HA	1:A:298:ARG:O	2.08	0.52
1:B:141:ARG:HD3	1:B:321:ARG:HH11	1.71	0.52
1:B:317:PHE:O	1:B:321:ARG:HG3	2.10	0.52
1:B:364:THR:O	1:B:368:ILE:HG13	2.09	0.52
1:A:162:ARG:HG3	1:A:162:ARG:HH11	1.74	0.52
1:B:432:LYS:HE3	1:B:432:LYS:HA	1.90	0.52
1:A:98:ILE:HD12	1:A:98:ILE:N	2.25	0.52
1:B:241:MSE:CE	1:B:283:ILE:HD12	2.38	0.52
1:A:99:ASP:OD1	1:A:102:LYS:HD2	2.10	0.52
1:A:453:THR:OG1	1:A:456:ILE:HG12	2.10	0.52
1:A:159:TYR:CZ	1:A:287:PRO:HB2	2.45	0.51
1:B:204:LYS:HE3	4:B:1078:HOH:O	2.08	0.51
1:B:341:PRO:HG3	1:B:401:MSE:HE2	1.92	0.51
1:A:426:LEU:C	1:A:428:GLY:N	2.64	0.51
1:B:368:ILE:CD1	1:B:442:ILE:HD12	2.40	0.51
1:B:112:ILE:HG12	1:B:116:LEU:HD23	1.91	0.51
1:A:206:LEU:C	1:A:206:LEU:HD12	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:PRO:HG2	1:B:401:MSE:HB3	1.91	0.51
1:B:233:PHE:CZ	1:B:235:PHE:HB3	2.45	0.51
1:A:129:HIS:CD2	3:A:602:GOL:H31	2.45	0.50
1:A:141:ARG:HG3	1:A:334:LEU:HD12	1.93	0.50
1:A:173:HIS:O	1:A:176:PRO:HD2	2.12	0.50
1:B:326:ARG:HH11	1:B:326:ARG:HG3	1.76	0.50
1:A:412:LYS:O	1:A:416:ILE:HG13	2.11	0.50
1:A:429:GLU:OE1	1:A:432:LYS:HG3	2.12	0.50
1:A:444:GLU:HB3	1:A:448:ARG:NH1	2.26	0.50
1:A:172:GLY:O	1:A:175:ILE:HG12	2.12	0.49
1:A:177:PHE:CE1	1:A:222:ILE:HD12	2.47	0.49
1:A:372:VAL:HG12	1:A:431:LYS:HB3	1.94	0.49
1:A:103:LEU:HD23	1:A:311:ILE:HD13	1.93	0.49
1:A:206:LEU:CD1	1:A:211:ALA:HB2	2.42	0.49
1:A:283:ILE:N	1:A:283:ILE:HD12	2.27	0.49
1:A:383:THR:HG22	1:A:386:GLU:OE1	2.12	0.49
1:B:143:MSE:HE3	1:B:146:VAL:CB	2.36	0.49
1:B:228:ASP:CB	1:B:231:LYS:HE2	2.42	0.49
1:A:231:LYS:HG2	1:A:468:PHE:CE1	2.47	0.49
1:A:86:ASP:OD2	1:A:88:TRP:HE3	1.96	0.49
1:B:133:ARG:O	1:B:134:ARG:HG3	2.13	0.49
1:B:139:SER:OG	1:B:336:HIS:HB2	2.13	0.49
1:A:182:TRP:O	1:A:186:VAL:HG22	2.13	0.49
1:A:449:ARG:HH11	1:A:449:ARG:HG2	1.78	0.49
1:A:262:GLN:O	1:A:266:ILE:HG12	2.13	0.48
1:B:112:ILE:CB	1:B:138:PHE:O	2.61	0.48
1:B:321:ARG:HB3	1:B:331:LYS:HE2	1.95	0.48
1:A:87:PRO:HD3	1:A:315:PRO:HG2	1.94	0.48
1:A:369:LYS:HG3	1:A:370:THR:N	2.28	0.48
1:B:149:ALA:HA	1:B:154:LYS:HE3	1.96	0.48
1:A:199:GLU:HB2	1:A:280:PHE:CE1	2.48	0.48
1:A:395:ASP:O	1:A:401:MSE:HE3	2.13	0.48
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.78	0.48
1:B:228:ASP:HB3	1:B:231:LYS:HE2	1.96	0.48
1:B:98:ILE:HG23	1:B:99:ASP:N	2.29	0.48
1:B:143:MSE:CE	1:B:146:VAL:HB	2.38	0.48
1:A:97:GLY:HA2	1:A:346:ALA:O	2.14	0.48
1:A:280:PHE:HA	1:A:283:ILE:HD13	1.95	0.48
1:A:95:ALA:HA	1:A:347:GLN:HE21	1.75	0.47
1:A:170:HIS:ND1	1:A:350:MSE:SE	2.97	0.47
1:A:384:ILE:O	1:A:388:ARG:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ARG:HH21	1:B:426:LEU:HD11	1.79	0.47
1:A:119:ARG:HG2	1:A:147:LEU:HD13	1.95	0.47
1:A:318:ARG:HB3	4:A:1041:HOH:O	2.13	0.47
1:B:384:ILE:HG23	1:B:385:GLU:CD	2.38	0.47
1:B:149:ALA:O	1:B:154:LYS:HB2	2.15	0.47
1:B:104:ILE:CG2	4:B:1080:HOH:O	2.57	0.47
1:A:138:PHE:H	1:A:138:PHE:HD2	1.61	0.47
1:A:196:THR:HB	1:A:199:GLU:HB3	1.96	0.47
1:A:314:ASP:N	1:A:315:PRO:CD	2.78	0.47
1:B:435:ILE:O	1:B:439:GLN:HG3	2.14	0.47
1:A:428:GLY:O	1:A:429:GLU:C	2.57	0.47
1:B:104:ILE:HG23	1:B:105:VAL:N	2.29	0.46
1:B:393:ASN:OD1	1:B:395:ASP:HB2	2.15	0.46
1:B:394:CYS:HB3	1:B:400:PHE:CD2	2.51	0.46
1:A:259:THR:OG1	1:A:262:GLN:HG3	2.15	0.46
1:B:184:GLN:HE22	1:B:227:PHE:HD1	1.64	0.46
1:A:169:MSE:HG3	1:A:361:LEU:HD22	1.97	0.46
1:B:100:TYR:CD1	1:B:103:LEU:HD12	2.50	0.46
1:B:283:ILE:O	1:B:287:PRO:HD3	2.15	0.46
1:A:418:LYS:HB2	1:A:418:LYS:HZ2	1.78	0.46
1:B:381:ARG:HG3	1:B:386:GLU:O	2.16	0.45
1:A:426:LEU:O	1:A:427:THR:C	2.59	0.45
1:A:100:TYR:CZ	1:A:338:THR:HB	2.51	0.45
1:A:207:THR:H	1:A:210:GLN:NE2	2.15	0.45
1:B:104:ILE:HG23	1:B:105:VAL:HG13	1.99	0.45
1:B:401:MSE:O	1:B:404:THR:OG1	2.33	0.45
1:B:300:ARG:HG2	1:B:300:ARG:NH1	2.27	0.45
1:A:206:LEU:HD11	1:A:211:ALA:HB2	1.99	0.45
1:A:201:TYR:HE1	3:A:601:GOL:HO2	1.62	0.45
1:A:259:THR:HA	1:B:274:CYS:HA	1.99	0.45
1:A:372:VAL:O	1:A:376:ALA:HB3	2.16	0.45
1:B:163:GLY:HA3	1:B:200:LYS:HE2	1.99	0.45
1:B:184:GLN:NE2	1:B:227:PHE:HD1	2.15	0.45
1:B:311:ILE:HG23	1:B:312:ASP:N	2.31	0.45
1:A:435:ILE:O	1:A:439:GLN:HG3	2.17	0.45
1:B:98:ILE:HG23	1:B:99:ASP:H	1.82	0.45
1:B:414:GLU:OE2	1:B:417:ARG:NH2	2.51	0.44
1:A:139:SER:HB3	1:A:336:HIS:HB2	1.99	0.44
1:A:216:VAL:O	1:A:219:ALA:HB3	2.18	0.44
1:A:100:TYR:O	1:A:101:ASP:CB	2.66	0.44
1:A:114:LYS:HE3	1:A:114:LYS:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ALA:HB3	2:A:501:TYM:O2'	2.18	0.44
1:B:136:ILE:O	1:B:337:SER:HA	2.17	0.44
1:A:307:ILE:HD13	1:A:317:PHE:CE1	2.52	0.44
1:A:218:ASN:N	1:A:218:ASN:HD22	2.16	0.44
1:A:349:LYS:HB2	2:A:501:TYM:N6	2.32	0.44
1:A:274:CYS:HB2	1:B:255:GLN:O	2.18	0.43
1:B:104:ILE:CD1	1:B:139:SER:HB3	2.47	0.43
1:A:339:PHE:O	1:A:341:PRO:HD3	2.18	0.43
1:A:207:THR:OG1	1:A:210:GLN:HG3	2.19	0.43
1:A:397:ASP:OD1	1:A:399:SER:HB2	2.18	0.43
1:A:403:LEU:HD21	1:A:434:LEU:HA	2.00	0.43
1:A:130:HIS:CD2	1:A:130:HIS:H	2.37	0.43
1:B:260:PHE:CE2	1:B:264:LYS:HD2	2.54	0.43
1:A:228:ASP:OD1	1:A:231:LYS:HE3	2.19	0.43
1:B:142:ASP:OD1	1:B:321:ARG:NH2	2.52	0.43
1:B:314:ASP:N	1:B:315:PRO:CD	2.82	0.43
1:A:165:SER:CB	1:A:168:ALA:HB3	2.49	0.43
1:B:373:ASN:HD21	1:B:432:LYS:HE2	1.84	0.43
1:B:388:ARG:NH2	1:B:426:LEU:HD11	2.34	0.43
1:A:103:LEU:CD2	1:A:311:ILE:HD13	2.49	0.43
1:A:165:SER:HB3	1:A:168:ALA:HB3	2.01	0.43
1:B:412:LYS:O	1:B:416:ILE:HG13	2.18	0.43
1:A:191:LEU:HD23	1:A:232:THR:HG23	2.00	0.42
1:A:162:ARG:HG3	2:A:501:TYM:O1P	2.18	0.42
1:A:360:PHE:C	1:A:362:THR:H	2.26	0.42
1:B:326:ARG:HG3	1:B:326:ARG:NH1	2.34	0.42
1:A:101:ASP:HA	1:A:104:ILE:HD12	2.01	0.42
1:A:167:GLU:O	1:A:168:ALA:O	2.37	0.42
1:B:104:ILE:CG2	1:B:105:VAL:N	2.82	0.42
1:B:160:THR:O	1:B:193:ILE:HA	2.19	0.42
1:A:160:THR:O	1:A:193:ILE:HA	2.19	0.42
1:B:216:VAL:O	1:B:219:ALA:HB3	2.19	0.42
1:B:250:ASN:ND2	1:B:291:ASN:ND2	2.55	0.42
1:B:98:ILE:O	1:B:99:ASP:HB3	2.20	0.42
1:A:162:ARG:HG3	1:A:162:ARG:NH1	2.35	0.42
1:A:92:THR:HG23	1:A:347:GLN:HA	2.02	0.42
1:B:291:ASN:HD22	1:B:291:ASN:C	2.28	0.41
1:B:300:ARG:NH2	1:B:302:ASP:OD2	2.53	0.41
1:A:138:PHE:CD2	1:A:138:PHE:N	2.86	0.41
1:B:104:ILE:HD11	1:B:110:SER:C	2.45	0.41
1:B:391:GLY:HA3	1:B:421:THR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLN:H	1:A:344:GLN:CD	2.28	0.41
1:B:164:PRO:HG3	1:B:195:MSE:HE3	2.01	0.41
1:A:162:ARG:NE	1:A:218:ASN:OD1	2.45	0.41
1:A:414:GLU:OE2	1:A:417:ARG:NH1	2.52	0.41
1:B:360:PHE:C	1:B:362:THR:H	2.28	0.41
1:A:218:ASN:O	1:A:222:ILE:HG12	2.21	0.41
1:B:399:SER:HA	1:B:434:LEU:HD22	2.03	0.41
1:B:170:HIS:HA	1:B:360:PHE:HA	2.02	0.41
1:B:344:GLN:HE21	1:B:344:GLN:HB2	1.67	0.41
1:A:100:TYR:C	1:A:102:LYS:N	2.76	0.41
1:B:240:TYR:HA	1:B:243:MSE:HG2	2.03	0.41
1:A:313:GLN:O	1:A:317:PHE:CD2	2.74	0.41
1:B:368:ILE:HD13	1:B:442:ILE:HD12	2.02	0.41
1:A:290:SER:HB3	1:A:303:ILE:HB	2.02	0.40
1:A:125:GLY:O	1:A:126:GLN:HG2	2.21	0.40
1:B:367:GLN:O	1:B:371:LYS:HG2	2.21	0.40
1:B:104:ILE:HD12	1:B:109:SER:HG	1.83	0.40
1:B:115:GLU:OE1	1:B:115:GLU:O	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/437 (88%)	360 (93%)	20 (5%)	6 (2%)	7	3
1	B	358/437 (82%)	336 (94%)	18 (5%)	4 (1%)	11	7
All	All	744/874 (85%)	696 (94%)	38 (5%)	10 (1%)	9	5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ALA
1	A	381	ARG
1	A	429	GLU
1	A	355	PRO
1	B	134	ARG
1	B	343	LEU
1	A	467	SER
1	B	303	ILE
1	B	372	VAL
1	A	87	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/369 (93%)	332 (97%)	11 (3%)	34	35
1	B	320/369 (87%)	315 (98%)	5 (2%)	55	62
All	All	663/738 (90%)	647 (98%)	16 (2%)	43	47

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	A	114	LYS
1	A	195	MSE
1	A	204	LYS
1	A	229	ILE
1	A	236	SER
1	A	295	GLN
1	A	335	LEU
1	A	417	ARG
1	A	418	LYS
1	A	430	LEU
1	B	236	SER
1	B	239	ASP
1	B	291	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	344	GLN
1	B	432	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	118	ASN
1	A	126	GLN
1	A	130	HIS
1	A	144	ASN
1	A	152	ASN
1	A	184	GLN
1	A	210	GLN
1	A	255	GLN
1	A	356	ASN
1	A	373	ASN
1	A	375	HIS
1	A	389	GLN
1	A	446	GLN
1	B	118	ASN
1	B	126	GLN
1	B	130	HIS
1	B	173	HIS
1	B	257	HIS
1	B	261	ASN
1	B	291	ASN
1	B	344	GLN
1	B	356	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	602	-	5,5,5	0.33	0	5,5,5	1.94	3 (60%)
3	GOL	A	601	-	5,5,5	0.39	0	5,5,5	1.96	3 (60%)
2	TYM	A	501	-	40,41,41	1.02	3 (7%)	58,61,61	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	A	601	-	-	3/4/4/4	-
2	TYM	A	501	-	-	1/21/39/39	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	TYM	CE3-CD2	2.82	1.44	1.39
2	A	501	TYM	CH2-CZ3	2.36	1.43	1.38
2	A	501	TYM	CZ2-CE2	2.29	1.43	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	GOL	C3-C2-C1	2.78	121.99	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	GOL	C3-C2-C1	2.55	121.13	111.80
3	A	602	GOL	O2-C2-C1	2.52	119.61	109.18
3	A	601	GOL	O2-C2-C1	2.45	119.32	109.18
3	A	602	GOL	O2-C2-C3	2.43	119.26	109.18
3	A	601	GOL	O2-C2-C3	2.30	118.69	109.18

There are no chirality outliers.

All (6) torsion outliers are listed below:

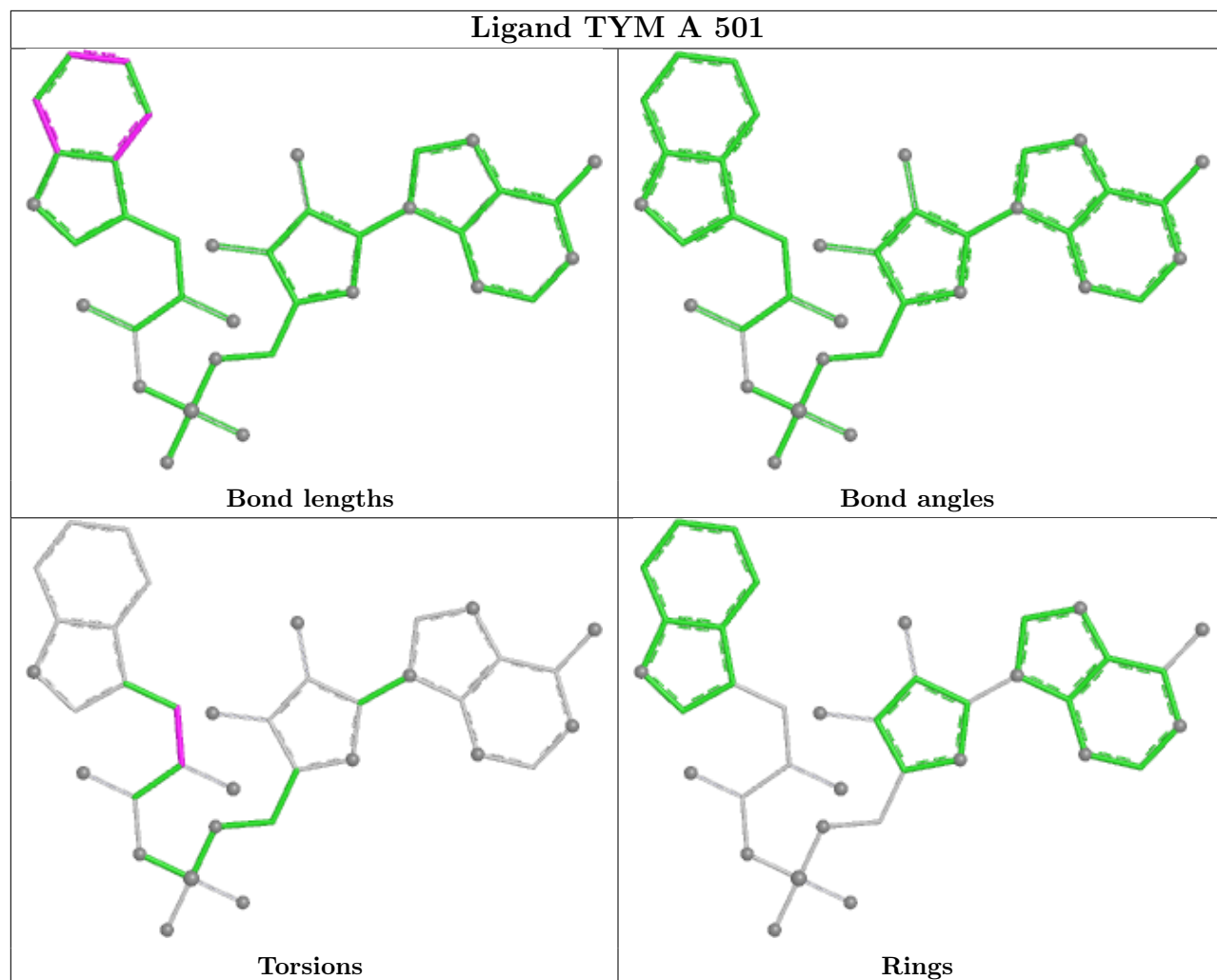
Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	A	601	GOL	O1-C1-C2-C3
3	A	601	GOL	O2-C2-C3-O3
3	A	601	GOL	O1-C1-C2-O2
2	A	501	TYM	NH3-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	GOL	1	0
3	A	601	GOL	1	0
2	A	501	TYM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	378/437 (86%)	1.23	85 (22%) 2 2	22, 49, 75, 84	11 (2%)
1	B	353/437 (80%)	1.19	83 (23%) 2 2	20, 51, 77, 88	6 (1%)
All	All	731/874 (83%)	1.21	168 (22%) 2 2	20, 50, 75, 88	17 (2%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	ILE	8.6
1	A	168	ALA	6.7
1	B	98	ILE	5.7
1	A	97	GLY	5.6
1	B	97	GLY	4.9
1	A	390	PHE	4.9
1	A	95	ALA	4.8
1	B	105	VAL	4.6
1	A	392	GLY	4.6
1	B	343	LEU	4.5
1	B	104	ILE	4.4
1	A	105	VAL	4.2
1	A	298	ARG	4.1
1	B	147	LEU	4.1
1	B	164	PRO	4.1
1	B	393	ASN	4.0
1	A	381	ARG	4.0
1	A	358	SER	3.9
1	A	422	SER	3.9
1	A	104	ILE	3.8
1	B	100	TYR	3.8
1	B	384	ILE	3.8
1	B	110	SER	3.7
1	A	90	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	396	VAL	3.7
1	B	168	ALA	3.7
1	B	387	HIS	3.7
1	A	430	LEU	3.7
1	B	152	ASN	3.7
1	B	111	LYS	3.6
1	B	166	SER	3.6
1	B	311	ILE	3.6
1	B	385	GLU	3.5
1	B	112	ILE	3.5
1	A	102	LYS	3.5
1	B	153	LYS	3.5
1	A	383	THR	3.5
1	B	426	LEU	3.4
1	A	94	SER	3.4
1	B	151	GLU	3.4
1	B	355	PRO	3.4
1	B	135	GLY	3.3
1	A	360	PHE	3.3
1	A	352	ALA	3.3
1	A	103	LEU	3.2
1	A	391	GLY	3.2
1	A	355	PRO	3.2
1	B	413	LEU	3.1
1	A	353	SER	3.1
1	A	429	GLU	3.1
1	B	372	VAL	3.0
1	B	117	ILE	3.0
1	B	365	ALA	3.0
1	B	467	SER	3.0
1	A	87	PRO	3.0
1	B	422	SER	3.0
1	B	118	ASN	3.0
1	A	359	ILE	3.0
1	A	468	PHE	3.0
1	A	466	LEU	2.9
1	B	103	LEU	2.9
1	B	163	GLY	2.9
1	B	150	TYR	2.9
1	B	377	PHE	2.9
1	B	186	VAL	2.9
1	A	420	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	452	VAL	2.9
1	A	295	GLN	2.8
1	A	357	SER	2.8
1	A	108	GLY	2.8
1	A	167	GLU	2.8
1	B	437	VAL	2.8
1	A	428	GLY	2.8
1	A	424	ALA	2.8
1	B	433	ALA	2.8
1	B	383	THR	2.8
1	B	133	ARG	2.7
1	A	91	GLN	2.7
1	B	115	GLU	2.7
1	B	390	PHE	2.7
1	B	316	TYR	2.7
1	A	85	VAL	2.7
1	A	348	THR	2.7
1	A	427	THR	2.7
1	A	455	GLU	2.7
1	A	384	ILE	2.7
1	B	123	ALA	2.7
1	B	138	PHE	2.7
1	A	229	ILE	2.7
1	B	139	SER	2.6
1	B	435	ILE	2.6
1	B	144	ASN	2.6
1	B	418	LYS	2.6
1	A	365	ALA	2.6
1	A	311	ILE	2.5
1	A	349	LYS	2.5
1	A	393	ASN	2.5
1	B	119	ARG	2.5
1	A	421	THR	2.5
1	A	351	SER	2.5
1	A	107	PHE	2.5
1	A	339	PHE	2.5
1	A	217	GLU	2.5
1	B	107	PHE	2.5
1	A	314	ASP	2.5
1	A	224	ALA	2.5
1	B	155	PRO	2.5
1	A	361	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	269	PHE	2.5
1	B	149	ALA	2.4
1	A	96	LYS	2.4
1	A	387	HIS	2.4
1	B	108	GLY	2.4
1	A	88	TRP	2.4
1	B	361	LEU	2.4
1	B	409	ASP	2.4
1	B	165	SER	2.4
1	B	116	LEU	2.4
1	A	82	GLU	2.4
1	B	265	GLY	2.4
1	A	312	ASP	2.4
1	A	166	SER	2.4
1	B	394	CYS	2.4
1	B	344	GLN	2.3
1	A	165	SER	2.3
1	A	456	ILE	2.3
1	A	394	CYS	2.3
1	A	145	GLN	2.3
1	B	342	ALA	2.3
1	B	410	ASP	2.3
1	A	457	VAL	2.3
1	B	428	GLY	2.3
1	A	398	VAL	2.2
1	A	356	ASN	2.2
1	B	113	ASP	2.2
1	B	167	GLU	2.2
1	B	416	ILE	2.2
1	B	312	ASP	2.2
1	A	426	LEU	2.2
1	A	369	LYS	2.2
1	A	230	ASN	2.2
1	A	115	GLU	2.2
1	B	392	GLY	2.2
1	A	443	ALA	2.2
1	B	101	ASP	2.2
1	A	266	ILE	2.1
1	A	442	ILE	2.1
1	A	210	GLN	2.1
1	B	424	ALA	2.1
1	B	412	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	420	TYR	2.1
1	A	89	THR	2.1
1	B	442	ILE	2.1
1	A	372	VAL	2.1
1	A	100	TYR	2.1
1	A	92	THR	2.1
1	A	315	PRO	2.1
1	A	364	THR	2.1
1	B	148	ASP	2.1
1	A	388	ARG	2.1
1	B	381	ARG	2.1
1	B	359	ILE	2.1
1	B	146	VAL	2.1
1	B	455	GLU	2.0
1	A	136	ILE	2.0
1	B	187	PHE	2.0
1	B	415	GLN	2.0
1	B	301	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

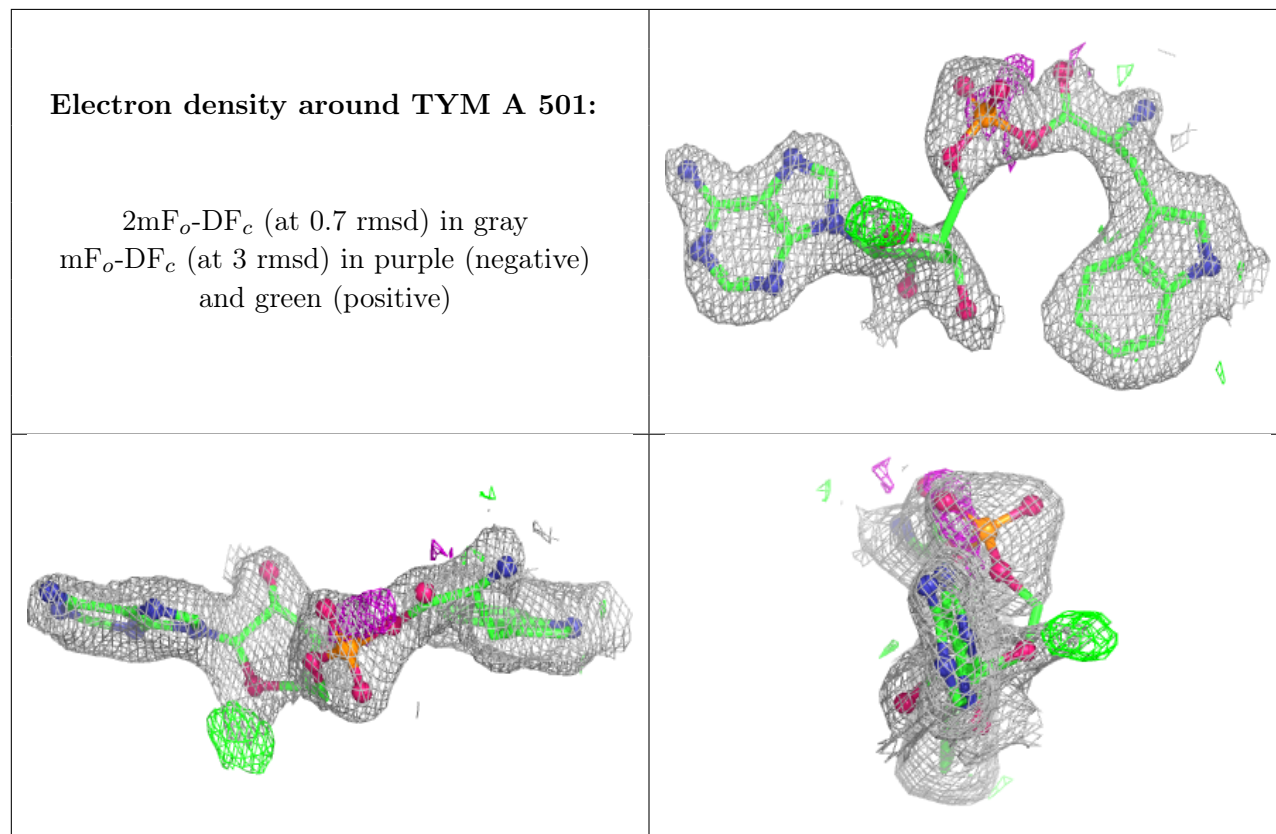
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	601	6/6	0.68	0.22	52,54,54,55	0
3	GOL	A	602	6/6	0.71	0.18	55,57,57,57	0
2	TYM	A	501	37/37	0.85	0.16	45,53,60,60	8

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.